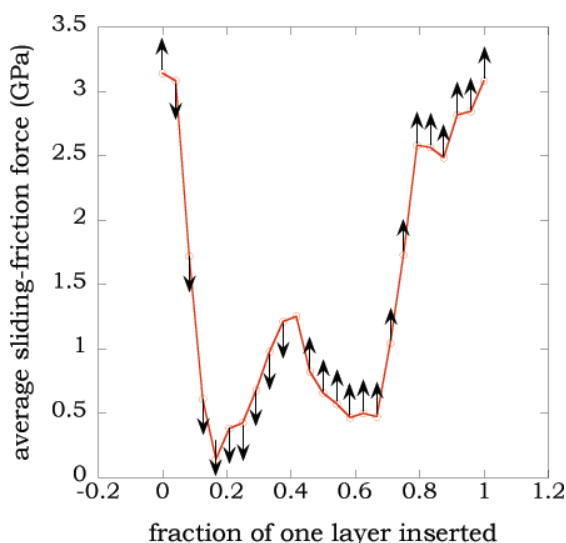


# Possible Self-healing in Tungsten under Fusion Reactor Conditions

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Radiation damage by fast neutrons due to fission and fusion can significantly degrade material properties. In a fusion reactor, long-lasting radiation-induced defects such as vacancies, vacancy clusters, and voids introduce additional nuclear safety complication in terms of trap sites for excessive tritium retention. This is especially true for the plasma-facing components of a fusion reactor like ITER, where extreme thermal stress is also present. Here we use molecular dynamics simulations to elucidate a self-healing mechanism in which the large thermal stress can facilitate the recombination of the neutron-collision-cascade-induced vacancies and interstitials through coupled grain boundary (GB) motion in body-centered-cubic (bcc) tungsten under fusion reactor conditions. Specifically, our simulations reveal that for a number of tungsten GBs, absorbing the fast-moving interstitials can help activate coupled GB motion at reduced mechanical stress; the migrating GB then sweeps up the less-mobile vacancies, facilitating vacancy-interstitial recombination inside the GB.

Fig. 1. Average sliding-friction force, under an applied shear strain, as a function of number of interstitials introduced into  $\Sigma 5(013)[100]$  grain boundary. The direction of normal grain boundary motion is indicated by the arrows. The points without arrows correspond to pure sliding.



A critical problem in developing fusion as a future energy source is designing materials that will tolerate the harsh radiation environment in a tokamak reactor. The challenges for tungsten (W), or any other plasma-facing component (PFC) in a fusion reactor, are compounded by the unusual combination of extensive radiation damage and strong mechanical stress. The neutrons produced in a fusion reactor can damage any structural material. The primary damage takes the form of interstitial atoms and vacancies. These defects and their aggregates

not only affect the mechanical, thermal, and electrical properties [1,2] of the PFC, but also introduce a number of additional nuclear safety concerns [3-5]. Healing of the material occurs when the vacancies and interstitials recombine and annihilate. In metals, however, the interstitials are highly mobile. They quickly diffuse to the nearest grain boundaries (GB) or surface, leaving the vacancies behind in the bulk of the material. Structural materials must be designed such that they tolerate the harsh radiation environment in a fusion reactor.

We have been studying the influence of radiation-induced damage on the GB sliding process in body-centered-cubic (bcc) W, employing atomistic computer simulations. For a number of GBs, we found the surprising result that introducing interstitials

or vacancies into the GB can reduce the average sliding-friction force under shear by more than an order of magnitude (see Fig. 1). Moreover, because these GBs typically shear in a well-known coupled way (linked sliding and normal migration) [6], we propose the following new self-healing mechanism for W under irradiation conditions. A collision cascade produces vacancies and highly mobile interstitials; the diffusing interstitials find, and are trapped at, a nearby GB. The interstitial-loaded GB is now so easy to shear that internal stresses in the crystal may set it in motion, sweeping up the vacancies close to the cascade center. Thus, under the right conditions, the very cascade that introduces damage into the material can initiate a mechanism that promotes healing of that damage. This mechanism is crucially dependent on the presence of a large mechanical stress, and the extreme stress conditions in a fusion reactor multiple gigapascal (GPa) appear to meet this requirement, at least during the plasma instabilities [7]. In our simulations we have also observed that the direction of normal GB motion switches to the opposite direction for many cases when the defects are introduced into the GB (e.g., see Fig. 1).

The self-healing phenomena under fusion reactor conditions can be illustrated by molecular dynamics simulations of a nanometer-scale W system with a  $\Sigma 5(013)[100]$  symmetric-tilt grain boundary. In the beginning of the simulation we introduce the interstitials into the GB and the vacancies into the upper grain (see Fig. 2). The sample is maintained at  $T = 1000$  K, which is the nominal operating temperature

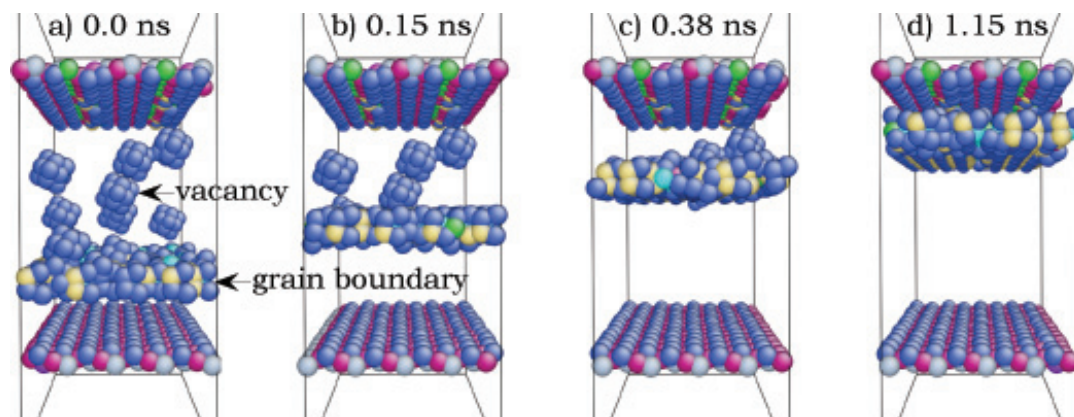


Fig. 2. Demonstration of the self-healing mechanism. A threshold stress for activation of the grain boundary motion is decreased with introduction of the interstitials into the grain boundary. The grain boundary migrates under an applied stress. It sweeps vacancies on its way up, leaving behind clean material without the defects. The top and bottom layers correspond to the free surfaces. The atoms are colored according to their coordination number, and bulk atoms are not shown.

of the PFC in a fusion reactor, and a shear stress of  $\sim 2$  Gpa is applied in the horizontal direction. Under these conditions, the  $\Sigma 5(013)[100]$  GB performs a coupled-normal migration plus parallel sliding-motion. The upward normal migration allows the GB to sweep up the bulk vacancies, which are largely immobile on the GB migration time scale. The healing of the radiation damage is evident as the sweeping GB leaves behind clean bulk W.

Experimentally, under irradiation, GBs have been observed to move in polycrystalline materials, as in electron-irradiated steel [8], and both void denuded zones [9] and segregant concentration profiles [10] have been observed to be asymmetrically distributed around GBs, consistent with GB motion. The observed reversal of the direction of GB motion as grains are traversed [8] might be reinterpreted in light of our results as a sign of a changing defect content.

Because GBs tend to act as efficient sinks for interstitials that are produced in collision cascades, and because interstitial loading enhances GB mobility as well as sometimes altering the coupling properties, we conclude that under the extreme stress conditions in a fusion reactor GB sweeping may contribute to radiation damage healing. Moreover, this mechanism may produce an effect even in systems where interstitials do not affect GB mobility, if the GB motion is coupled under

accessible mechanical stress. This sweeping mechanism illustrates the complexities associated with the atomic-scale interactions of point defects with GBs that may be crucial for understanding radiation damage evolution. It may contribute to the design of new structural materials for service in extreme environments, such as fusion reactors.

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